

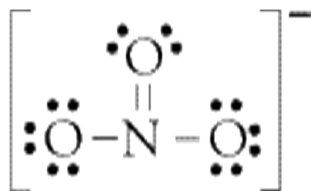
Name _____

AP Chemistry

Resonance & Formal Charge

Resonance Structures

On occasion, there can be more than one correct Lewis structure for a molecule. These different structures are known as resonance structures. Resonance is invoked when more than one valid Lewis structure can be written for a particular molecule. For example, a Lewis structure of NO_3^- could be drawn as



However, the double bond can appear in two other locations, giving two more structures:

The actual structure is an average of the resonance structures, in this case all three of them.

Example:

Write the Lewis structure for the nitrite ion (NO_2^-), including all resonance structures.

Formal Charge

There are often multiple Lewis structures for a single molecule. How do you tell which one is the most accurate to the actual bonding of the molecule? Formal charge can help evaluate which Lewis structure is the most accurate. It describes the difference between the number of

valence electrons on the free atom and the number of valence electrons assigned to the atom in the molecule.

$$\text{Formal Charge} = V - \left(L + \frac{1}{2} S \right)$$

V = # of valence electrons on the free atom

L = # of electrons present as lone pairs

S = # of shared electrons

When assigned the formal charge there are two assumptions made:

- (1) Lone pair electrons belong entirely to the atom in question.
- (2) Shared electrons are divided equally between the two sharing atoms.

The sum of the formal charges of all the atoms in a given molecule or ion must equal the overall charge on that species. To evaluate the Lewis structures based on the formal charge, it is assumed that atoms in the molecules try to achieve formal charges as close to zero as possible and any negative formal charges are expected to reside on the most electronegative atoms.

Example:

Give Lewis structures for the sulfate ion, SO_4^{2-} . Which structure or structures are most appropriate according to the formal charges?

Practice Questions:

- 1) The cyanate ion (NCO^-), like the thiocyanate ion, has three possible Lewis structures. Draw the three Lewis structures and assign formal charges to the atoms in each structure. Which Lewis structure is the preferred one?

2) Calculate the formal charge on the indicated atom in each of the following molecules or ions:

(a) The central oxygen atom in O_3

(b) Phosphorus in PF_6^-

(c) Nitrogen in NO_2

(d) Iodine in ICl_3

(e) Chlorine in HClO_4 (hydrogen bonded to O)

3) Some of the important in the atmosphere are ozone (O_3), sulfur dioxide, and sulfur trioxide. Write Lewis structures for these three molecules. There are two structures for the first two molecules and three for the last one.

4) Benzene (C_6H_6) consists of a six-membered ring of carbon atoms with one hydrogen bonded to each carbon. Write the Lewis structure for benzene. There are two structures for benzene.

5) Draw two equivalent structures for the formate ion, HCO_2^- .